# Quantum Belief Propagation

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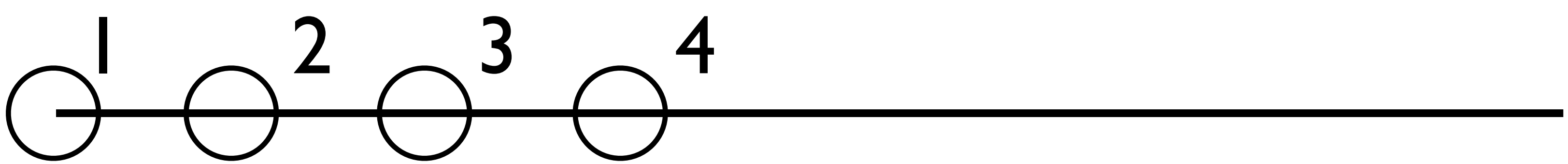
# Classical Belief Propagation: the transfer matrix

- Solve system of N sites, compute probability distribution of last site
- Add one more site and repeat




Discrete set of states on each site: $\sigma_i$

Nearest neighbor Hamiltonian: $H = \sum_i h_{i,i+1}$

Hamiltonian on first N sites: $h^{(N)} \equiv \sum_{i=1}^{N-1} h_{i,i+1}$

Partition function for chain of N sites:

$$Z^{(N)} = \sum_{\{\sigma_1,\ldots,\sigma_N\}} \exp(-\beta h^{(N)})$$

Probability distribution:

$$P^{(N)}(\sigma_1, ..., \sigma_N) = \frac{1}{Z^{(N)}} \exp(-\beta h^{(N)})$$

Probability of last site:

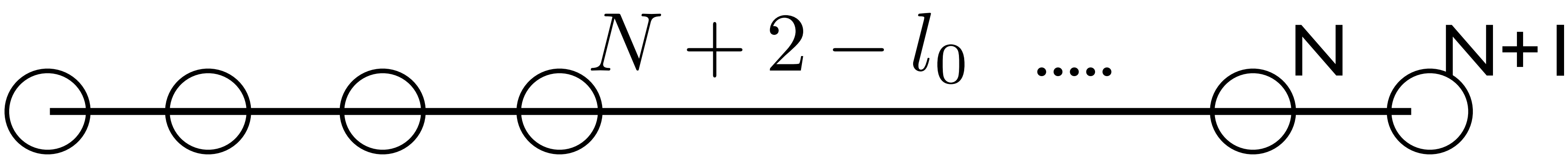
$$P^{(N)}(\sigma_N) = \sum_{\{\sigma_1,\ldots,\sigma_{N-1}\}} P^{(N)}(\sigma_1, ..., \sigma_N)$$

Recursion relation:

$$P^{(N+1)}(\sigma_{N+1}) \propto \sum_{\sigma_N} P^{(N)}(\sigma_N) \exp(-\beta h_{N,N+1})$$

# Quantum belief propagation:

- Analogue of probability on last site is reduced density matrix
- Need window of several sites. Window size is $l_0 - 1$

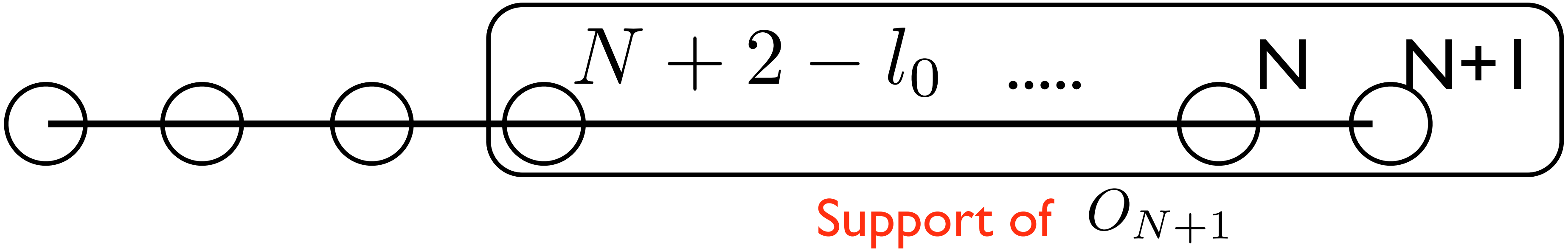



$$\rho^{(N)} = \exp(-\beta h^{(N)})$$

$$\rho_{red}^{(N)} = \mathrm{Tr}_{1,\ldots,N+1-l_0}(\rho^{(N)})$$

# Quantum belief propagation:

Construct O such that: $\rho^{(N+1)} \approx O_{N+1}\rho^{(N)}O_{N+1}^{\dagger}$




$$\rho^{(N+1)} = O_{N+1}O_N O_{N-1}\ldots O_{N-1}^{\dagger}O_N^{\dagger}O_{N+1}^{\dagger}$$

$$\rho_{red}^{(N+1)} = \mathrm{Tr}_{N+2-l_0}\left(O_{N+1}(\rho_{red}^{(N)} \otimes 1_{N+1})O_{N+1}^{\dagger}\right)$$

# Algorithm:

- Initialize reduced density matrix on first $l_0 - 1$ sites
- Iterate completely positive map until convergence
- Compute partition function from normalization
- Observables: insert operator before tracing on first site

Completely positive map:
$$\rho_{red} \to \mathrm{Tr}_1\Big(O_{N+1}(\rho_{red}^{(N)} \otimes 1_{N+1})O_{N+1}^\dagger\Big)$$

Observables:
$$\rho_{red} \to \mathrm{Tr}_1\Big(S_1^z O_{N+1}(\rho_{red}^{(N)} \otimes 1_{N+1})O_{N+1}^\dagger\Big)$$

# Performance:

- Computational effort : diagonalize operators of dimension $2^{l_0}$ to compute O.
- Window size needed scales as $l_0 \sim v_{LR}\beta$
- No Trotter error, very accurate at high temperature
- Handle disorder by precomputing operators.

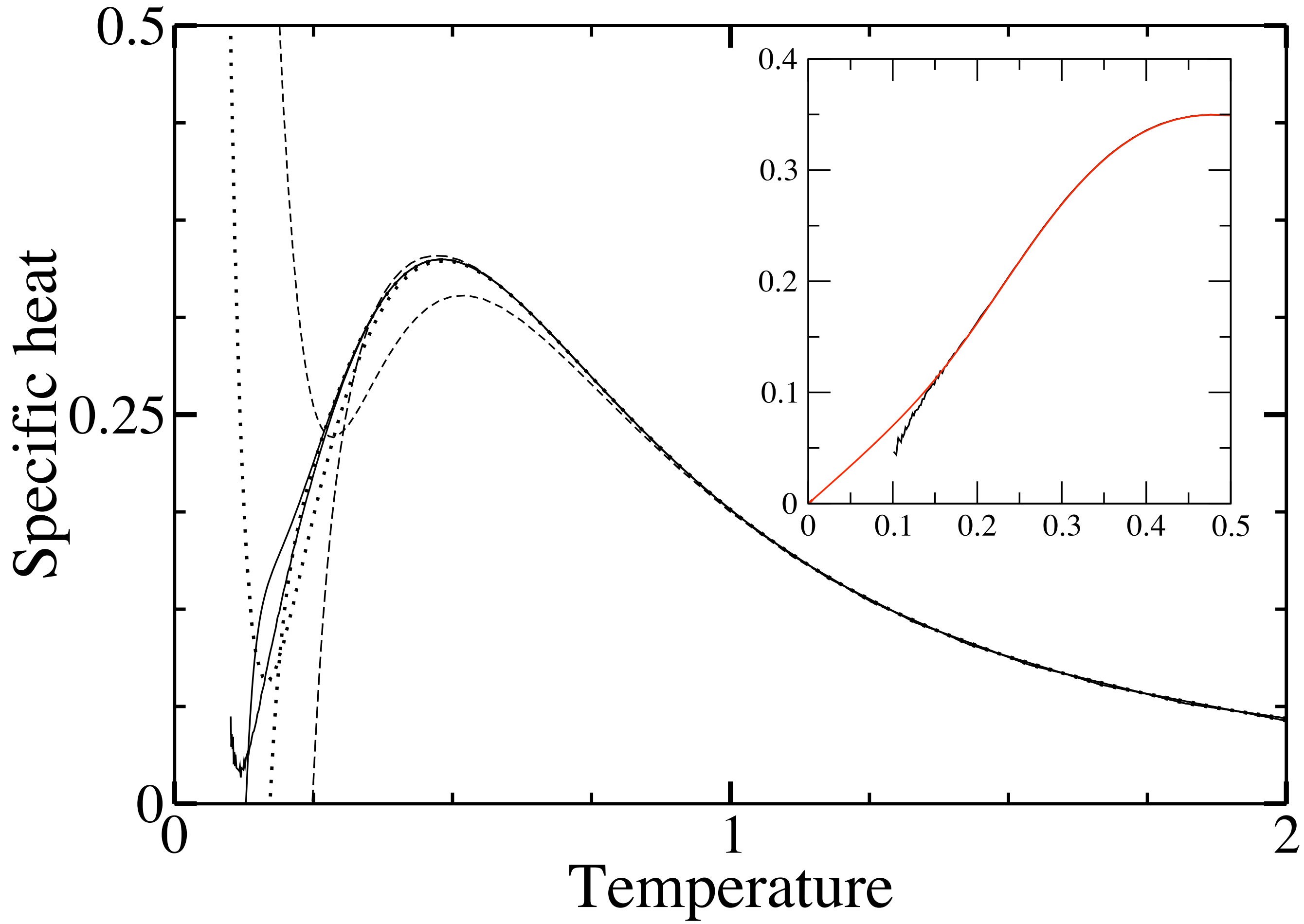
Heisenberg chain: $\chi_{exact}(T_{max}) = 0.146926279....$

$$\chi_{QBP}(T_{max}) = 0.146927031....$$

for 10-by-10 matrices diagonalized (<.1 second CPU time)

# Spin-1/2 Heisenberg Chain

$$H = \sum \vec{S}_i \cdot \vec{S}_{i+1}$$




thanks A. C. Klumper for data

FIG. 1: Specific heat against temperature for $l_0 = 3$ (dashed line),5 (dotted line), 7 (solid line). Curves that go negative are from $-3\beta^2\partial_\beta\langle S_i^z S_{i+1}^z\rangle$. while those that diverge positively are from $\beta^2\partial_\beta^2 \log(Z)$. Inset: $l_0 = 9$ and Bethe ansatz.

# Spin-1/2 disordered chain:

$$H = \sum_i J_i \vec{S}_i \cdot \vec{S}_{i+1} + \sum_i K_i \vec{S}_i \cdot \vec{S}_{i+2}$$



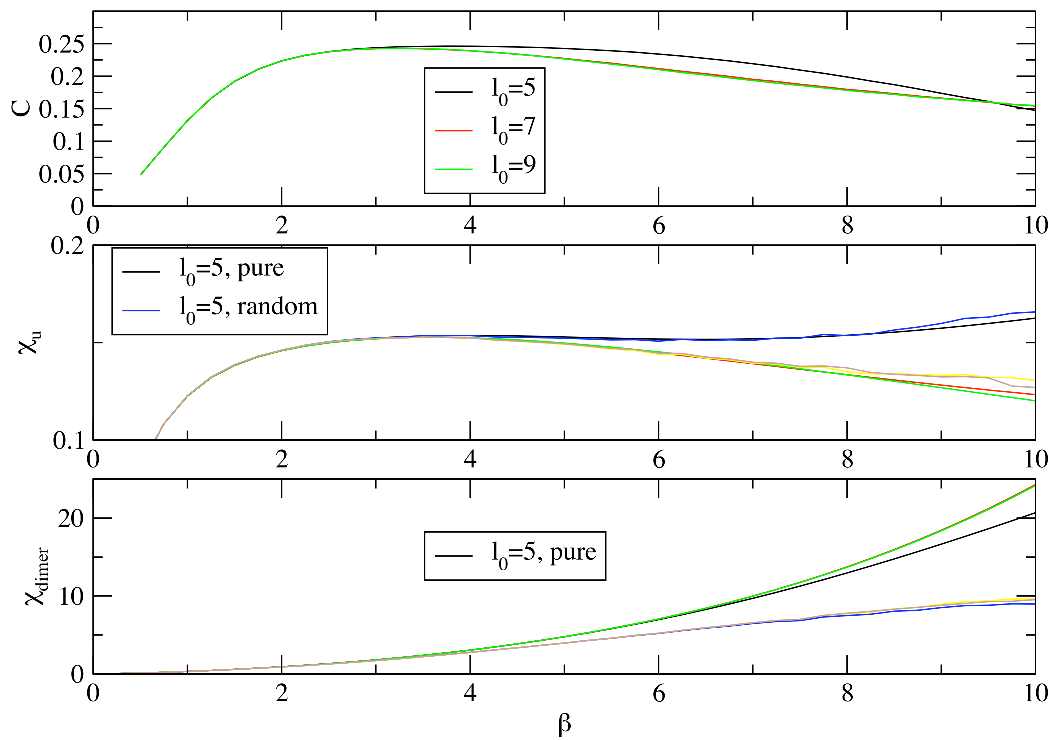



FIG. 1: Top: specific heat for the pure system. Middle: uniform susceptibility for the pure system ($l_0 = 5, 7, 9$ are black, red, green respectively) and the disordered system ($l_0 = 5, 7, 9$ are blue, yellow, brown respectively). Bottom: dimer susceptibility for the pure system ($l_0 = 5, 7, 9$ are black, red, green respectively) and the disordered system ($l_0 = 5, 7, 9$ are blue, yellow, brown respectively).

QBP Equations:

Exact result for small change in H:

$$\partial_s \exp[-\beta(H + sA)] = \eta_s \exp(-\beta H_s) + \exp(-\beta H_s)\eta_s^\dagger$$

$$\eta_s = -\int \mathrm{d}\omega \, (\frac{\beta}{2} + \beta F(\omega))A^{\omega,s}$$

classical term

quantum term

Perturbation at frequency omega

Integrate to add site:

$$O = \exp(\int_0^1 \mathrm{d}s \; \eta_s)$$

# Conclusions

- Accurate at high temperature
- Works well on loopless models
- Can we extend to loopy models?
- How do the different QBPs relate? (Poulin, Leifer)
- Works well for disorder by precomputing O
- A new kind of transfer matrix